Improved Heat Transfer Prediction for High-Speed Flows over Blunt Bodies using Adaptive Mixed-Element Unstructured Grids

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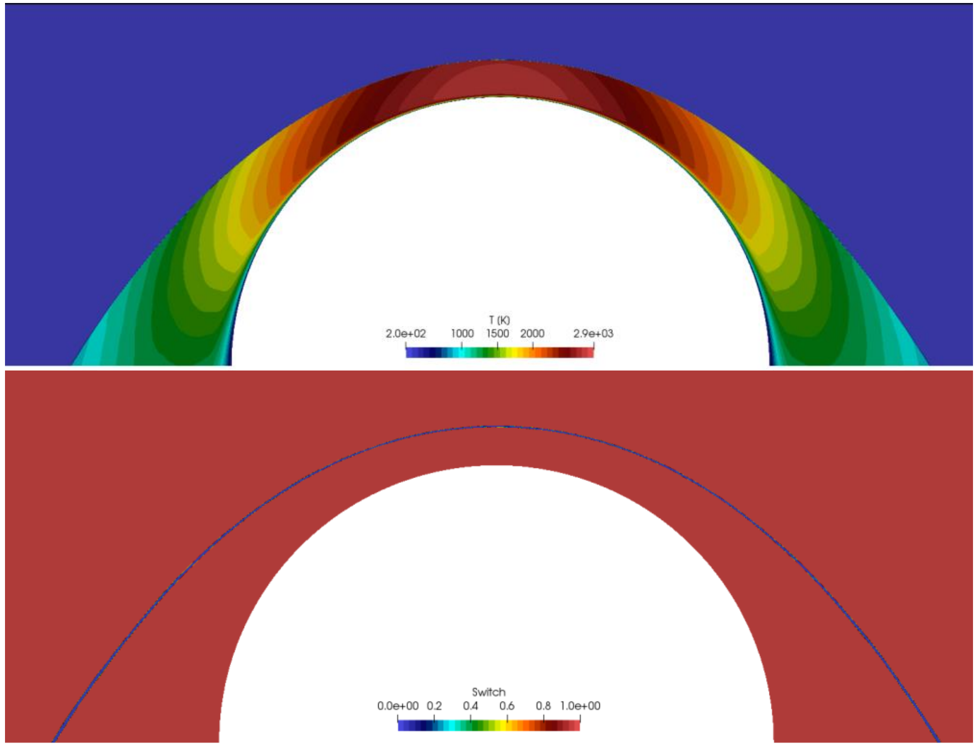
Motivation

- Design of atmospheric entry and hypersonic vehicles relies on accurate aerothermodynamic prediction. Various physical phenomena must be captured including:
  - Strong shocks
  - Shock-boundary layer interactions
  - Thermochemical nonequilibrium
- Current best practices for CFD are to create high-quality shock-aligned structured grids
- Unstructured grids have benefits over traditional structured grids
  - Complex geometry is more straightforward
  - Anisotropic and location-based refinement
- **This work will present algorithmic improvements and adaptive mesh refinement techniques to enable improved high-speed vehicle prediction using unstructured grids**

Introduction

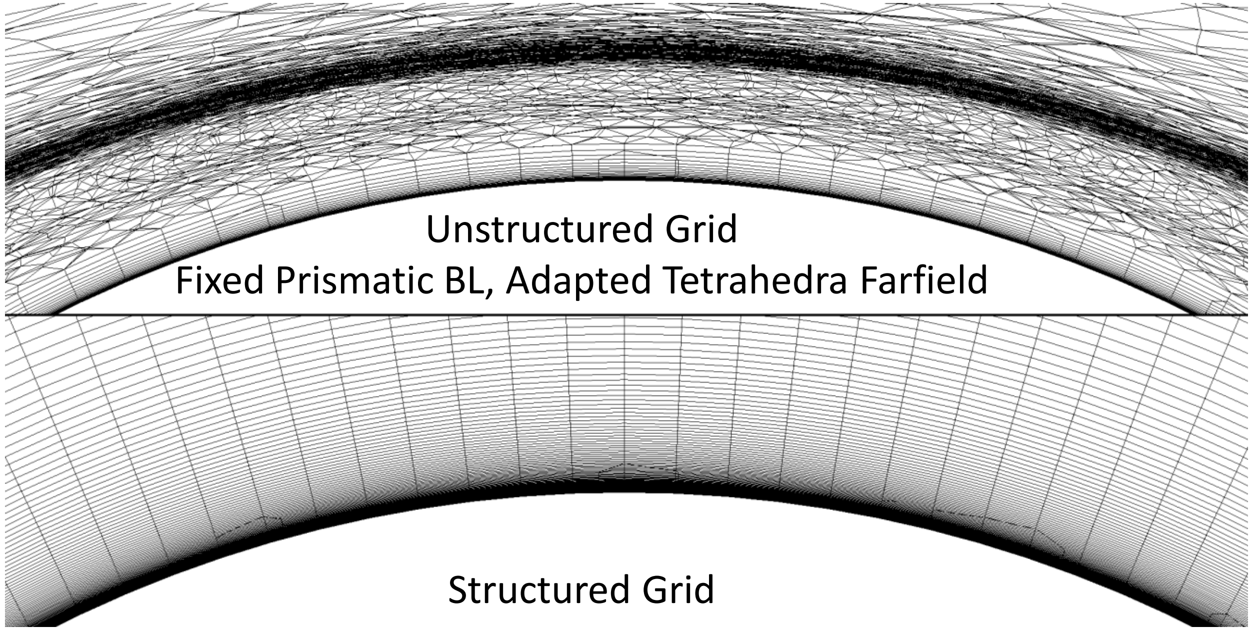
- An improved inviscid flux scheme, HLLE++, first implemented in NASA OVERFLOW, has been adapted and incorporated into NASA FUN3D
- Roe scheme exhibits issues for supersonic flows when grids are not adequately aligned with shocks
  - Requires an entropy fix to prevent nonphysical expansion shocks
  - Susceptible to carbuncles which requires eigenvalue fixes
    - Tuned values for specific problems → not ideal for automation
- HLLE++ is an adaptation of the Roe scheme:
  - Removes the need for an entropy fix
  - Reduces the susceptibility to carbuncles
  - More numerically dissipative algorithm around strong shocks
  - Incorporates an improved and stronger shock switch
- Some limiter improvements to reduce limiting near the wall were also found to be important
- **Please see paper for full details on algorithmic improvements**



Hypersonic ($M_\infty = 8$) flow over a sphere
Top: Slice of Temperature (K)
Bottom: Slice of Shock Switch

Introduction (cont.)

- Historically, prisms have been used for boundary layers (BLs)
- Ideally, shocks are captured in prismatic portions of the grids
- In this work, a small portion of the BL is captured using prisms, with adapted tetrahedra outside of this area to capture shock waves. Recent work[1] by Gao et al. demonstrated reasonable success using this approach with a stabilized Finite Element Method.
- NASA refine, historically only able to work with tetrahedra, has been adapted thanks to lead developer Mike Park to enable usage on mixed-element grids
- For this work, the surface grid and prismatic regions are fixed
    - These regions can be eventually automated and adapted using methods such as AFLR and strand meshing to enable eventual usage of a Sketch-to-Solution[2] process
    - A Sketch-to-Solution[2] process further automates the mesh generation process; the user provides a clean CAD geometry which is adapted based on the flow solution automatically



Note: minor plotting artifacts in structured regions due to visualization algorithm

[1]Gao, S., Seguin, J., Habashi, W. G., Isola, D., & Baruzzi, G. (2019). A finite element solver for hypersonic flows in thermo-chemical non-equilibrium, Part II. *International Journal of Numerical Methods for Heat & Fluid Flow*.

[2]Kleb, W. L., Park, M. A., Wood, W. A., Bibb, K. L., Thompson, K. B., & Gomez, R. J. (2019). Sketch-to-solution: An exploration of viscous CFD with automatic grids. In *AIAA Aviation 2019 Forum* (p. 2948).

Governing Equations and Numerical Implementation

- NASA FUN3D is the flow solver used for this work
- Node-based finite-volume approach on general unstructured grids
- Thermochemical Nonequilibrium (“Generic Gas”) path is used
- Conservation of species, momentum, energies, and turbulence variables
- Two-temperature model available for thermal nonequilibrium
- 2 equation models (e.g., SST), Spalart-Allmaras turbulence model with Catris-Aupoix compressibility correction; DES option
- Variable species, energies, and turbulence equations
- Fully implicit formulations are used to integrate the equations in time
    - Sparse block linear system: $A\boldsymbol{x} = \boldsymbol{b}$
    - Matrix A composed of diagonal and off-diagonal $N_{eq}\, x\, N_{eq}$ blocks
    - Memory and solution time increases as $O\left(N_{eq}^2\right)$
- System solved with multicolor point-implicit approach

$$\frac{\partial}{\partial t}(\rho y_s) + \frac{\partial}{\partial x_j}(\rho y_s u_j) - \frac{\partial}{\partial x_j}(J_{sj}) = \dot{\omega}_s$$

$$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}(\rho u_i u_j + p\delta_{ij}) - \frac{\partial}{\partial x_j}(\tau_{ij}) = 0$$

$$\frac{\partial}{\partial t}(\rho E) + \frac{\partial}{\partial x_j}\left((\rho E + p)u_j\right) - \frac{\partial}{\partial x_j}\left(u_k \tau_{kj} + \dot{q}_j + \sum_{s=1}^{N_s} h_s J_{sj}\right) = 0$$

$$\frac{\partial}{\partial t}(\rho E_v) + \frac{\partial}{\partial x_j}(\rho E_v u_j) - \frac{\partial}{\partial x_j}\left(\dot{q_V}_j + \sum_{s=1}^{N_s} h_{V_s} J_{sj}\right) = S_v$$

$$\frac{\partial}{\partial t}(\rho \tilde{\nu}) + \frac{\partial}{\partial x_j}(\rho \tilde{\nu} u_j) - \frac{\partial}{\partial x_j}\left(\frac{1}{\sigma}\left(\mu \frac{\partial \tilde{\nu}}{\partial x_j} + \sqrt{\rho}\tilde{\nu}\frac{\partial \sqrt{\rho}\tilde{\nu}}{\partial x_j}\right)\right) = S_{\tilde{\nu}}$$

$$\boldsymbol{q} = [\rho \vec{y}_s, \rho \vec{u}, \rho E, \rho E_v, \rho \tilde{\nu}]^T$$

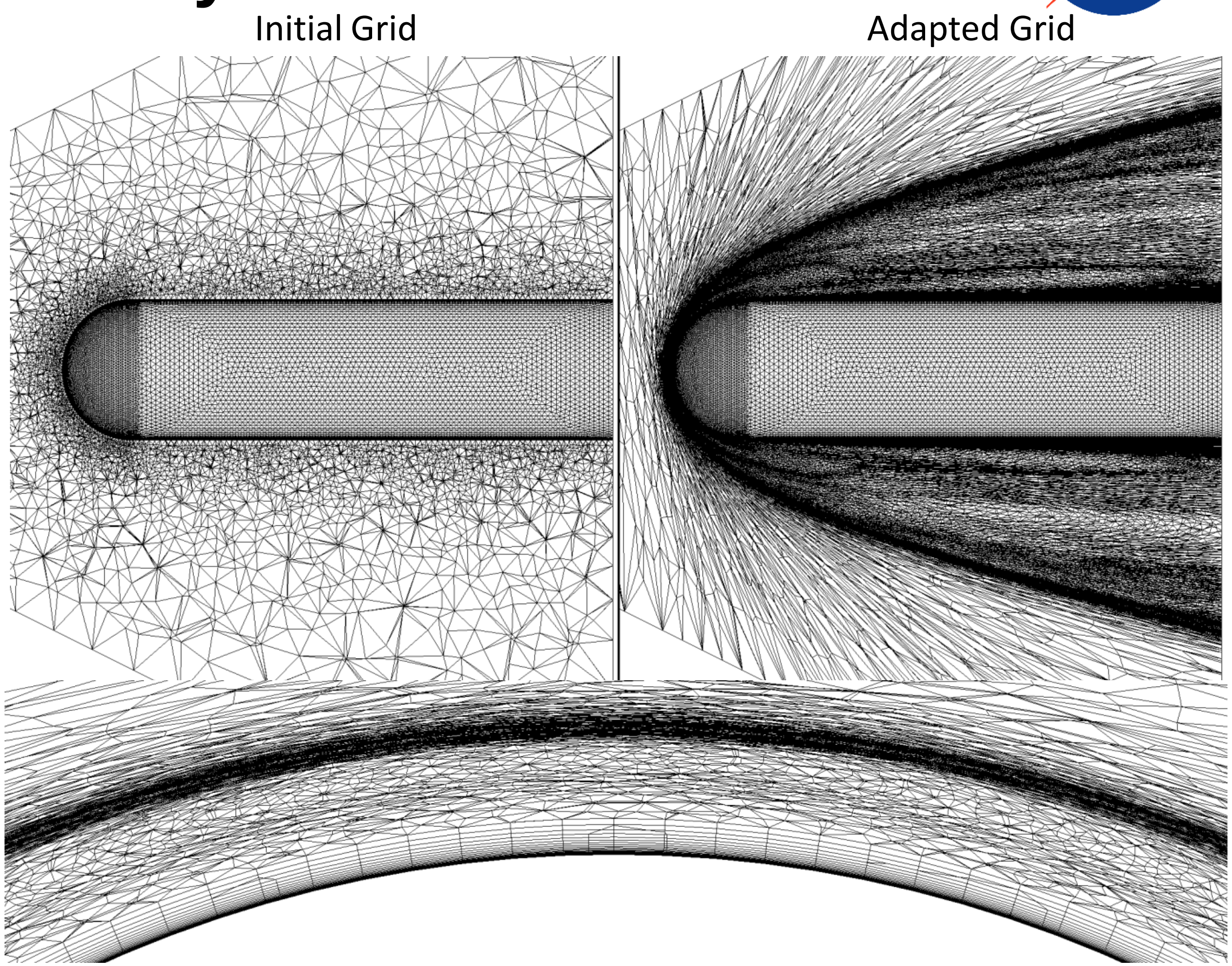
$$\int_{\boldsymbol{V}} \frac{\partial \boldsymbol{q}}{\partial t} dV + \oint_{\boldsymbol{S}} (\boldsymbol{F} \cdot \boldsymbol{n}) dS - \int_{\boldsymbol{V}} \boldsymbol{S} dV = \boldsymbol{0}$$

$$\left[\frac{V}{\Delta\tau}\boldsymbol{I} + \frac{V}{\Delta t}\boldsymbol{I} + \frac{\partial \widehat{\boldsymbol{R}}}{\partial \boldsymbol{q}}\right]\Delta\mathbf{q} = -\mathbf{R}(\mathbf{q}^{n+1,m}) - \frac{V}{\Delta t}(\mathbf{q}^{n+1,m} - \mathbf{q}^{\mathrm{n}})$$

$$\mathbf{q}^{n+1,m} = \mathbf{q}^{n+1,m} + \Delta\boldsymbol{q}$$

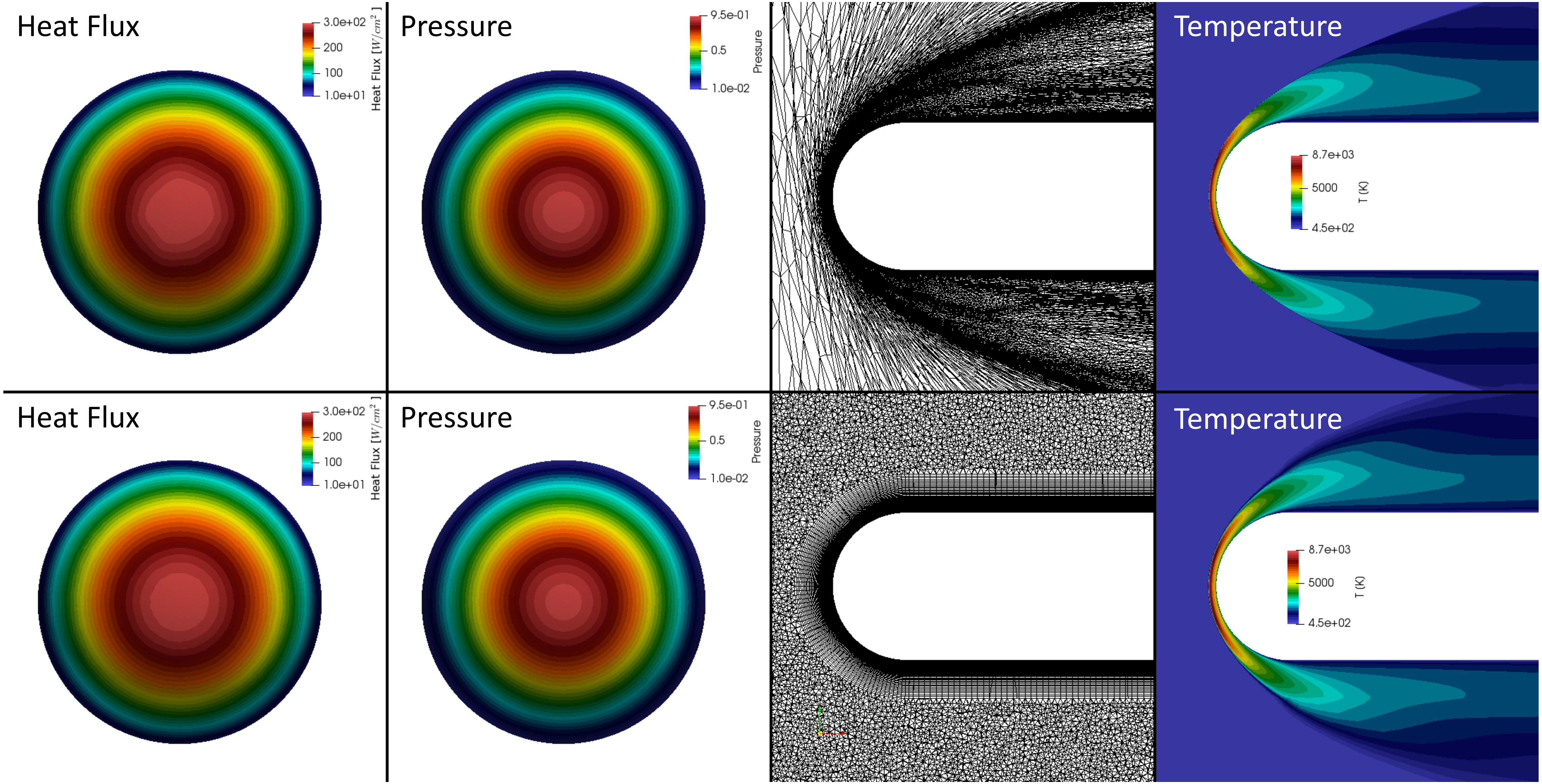
High Enthalpy Hypersonic Flow Around a Hemisphere Cylinder

- $M_\infty = 9.8, T_\infty = 450\ K, p_\infty = 230\ Pa, R = 0.0254\ m\ (1\ in)$
- 5 species air, two-temperature gas model
- Initial 3D (asymmetric) grid consists of 600k points, 400k tetrahedra, and 1m prisms
  - Prismatic BL with 40 layers generated
    - Last layer aspect ratio ~ 7
    - Surface properties and interface observed to be better predicted when aspect ratio is O(1-10)
- Process is as follows:
  - Initial solution is obtained on first grid
  - Grid is adapted based on translation/rotational temperature Hessian and target number of points outside of prismatic region
  - Previous solution is interpolated onto adapted grid for new initial condition
  - Process is repeated for N cycles
- Final grid consists of 4.6m points (target = 4m), 23.6m tetrahedra, and 1m prisms

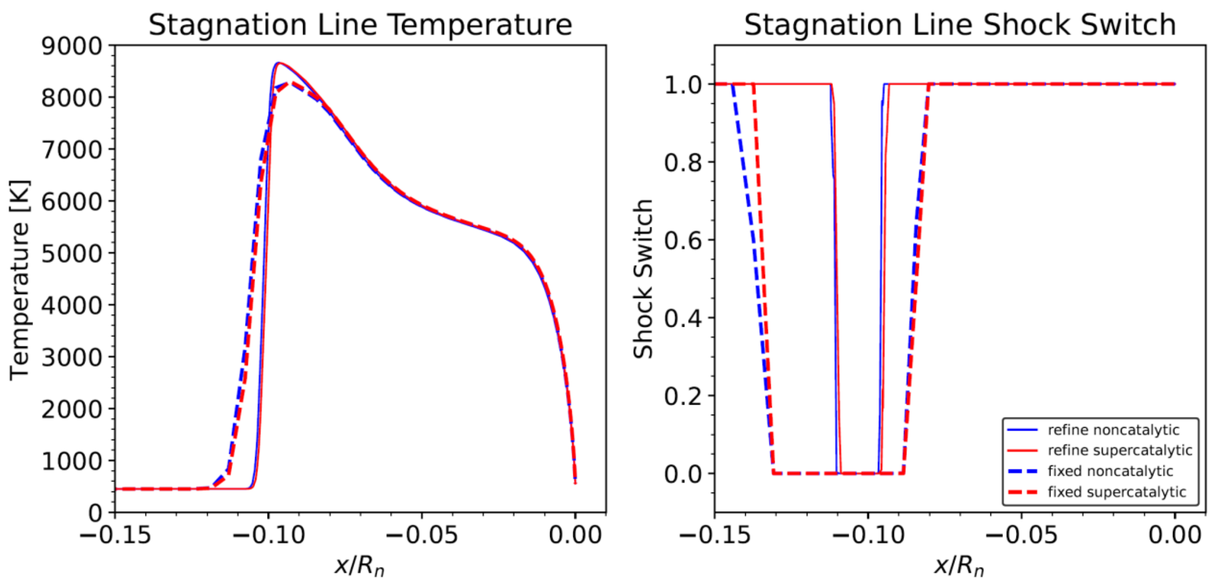


Note: minor plotting artifacts in structured regions due to visualization algorithm

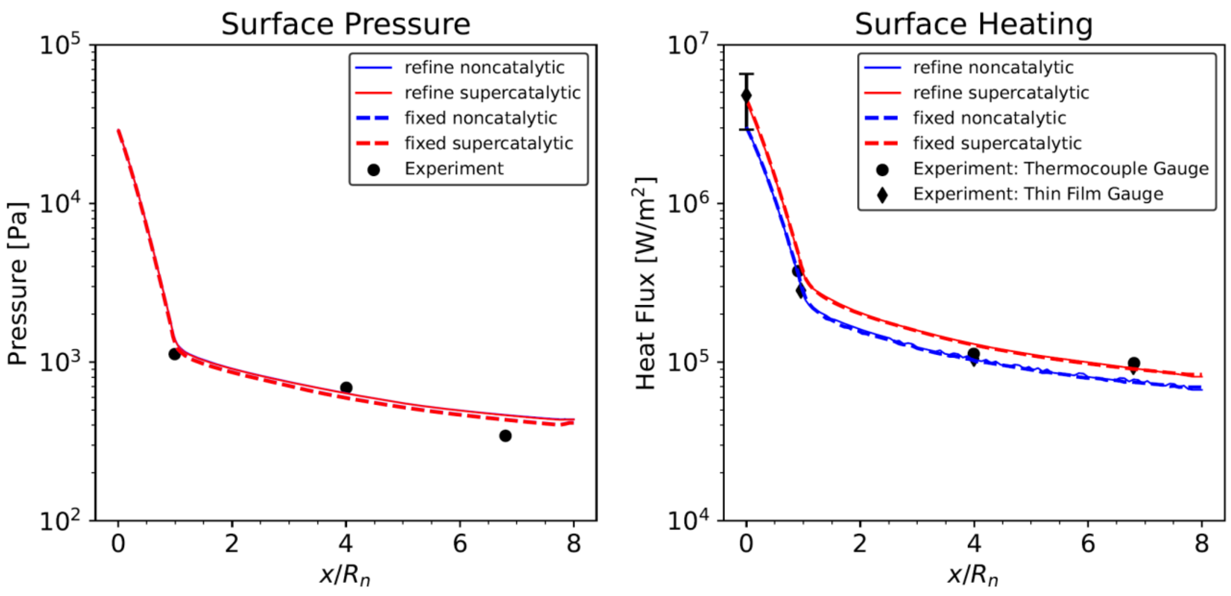
High Enthalpy Hypersonic Flow Around a Hemisphere Cylinder (cont.)



High Enthalpy Hypersonic Flow Around a Hemisphere Cylinder (cont.)



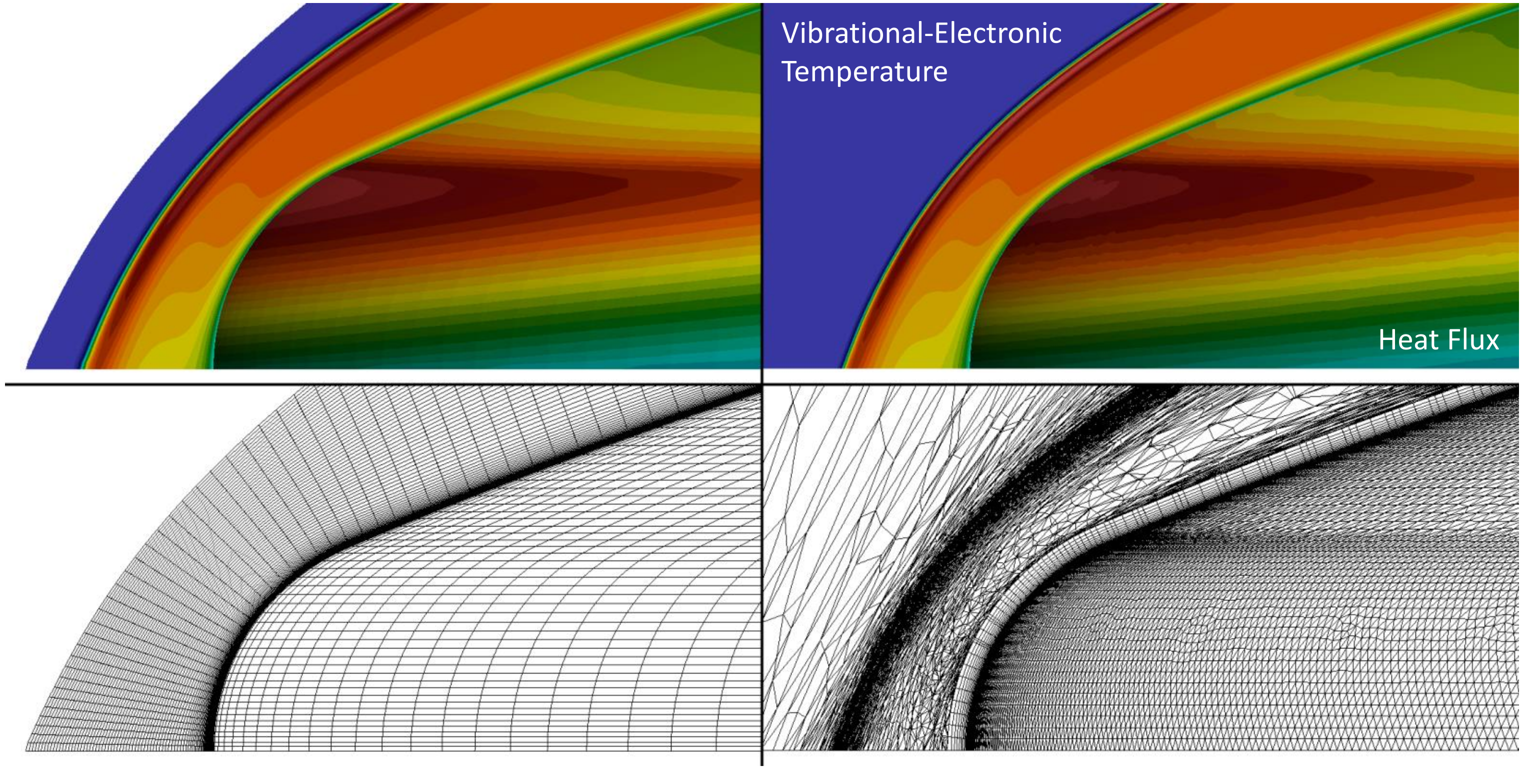
Peak shock temperature ∼400 Kelvin larger for adapted grid



Peak stagnation heat transfer within 0.1%, Drag within 1.5%

Hypersonic Flow over the Crew Exploration Vehicle

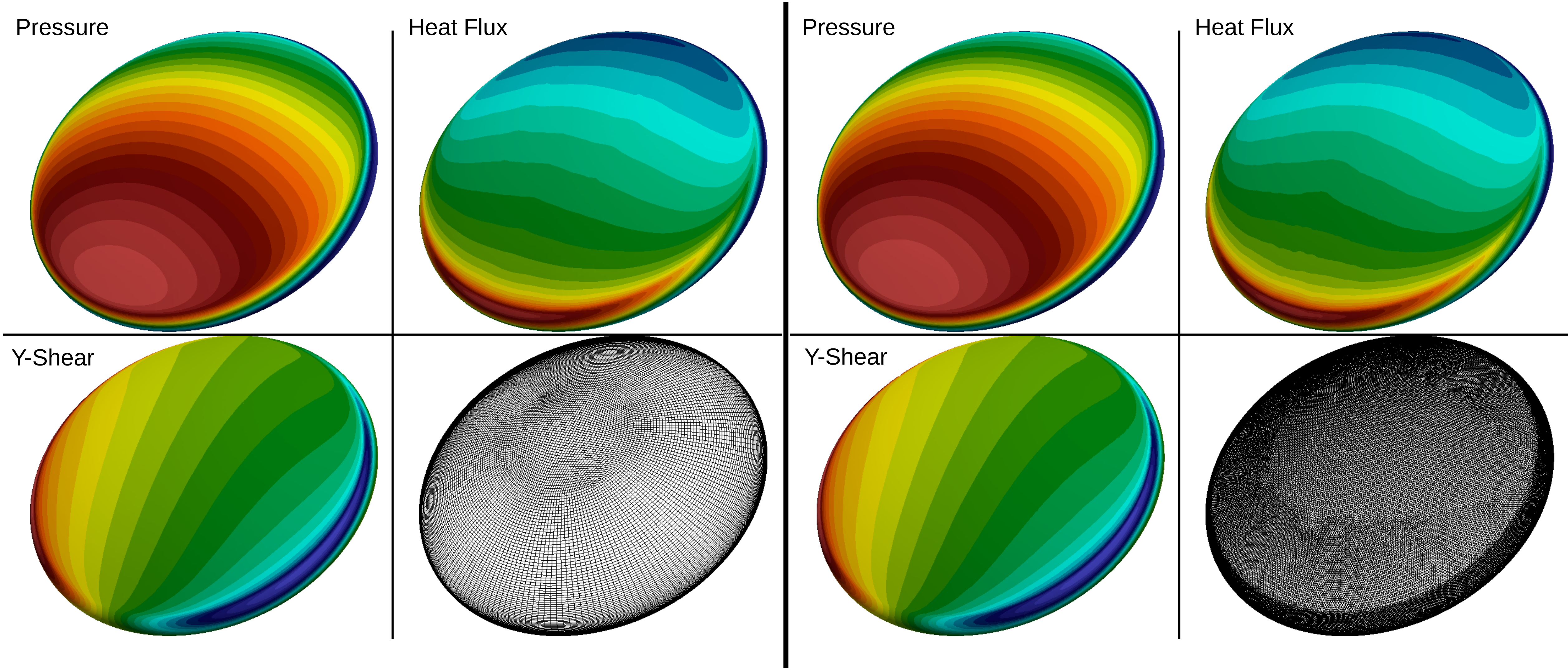
- Representative Earth reentry capsule
- $u_\infty = 10\,\frac{km}{s}$
- $M_\infty \approx 35$
- $\alpha = 28°$
- 11 species, two-temperature air model
- Structured grid composed of 1.6m points
- Unstructured grid composed of 3.1m points
- Surface spacing is comparable, but more isotropic for unstructured grid
- **In this work, iteration and grid point strategies have not been optimized**



Left: CEV structured grid results. Right: CEV unstructured adapted grid results. Top contours depict centerline Vibrational-Electronic Temperature in the flow field and heat flux on the surface.

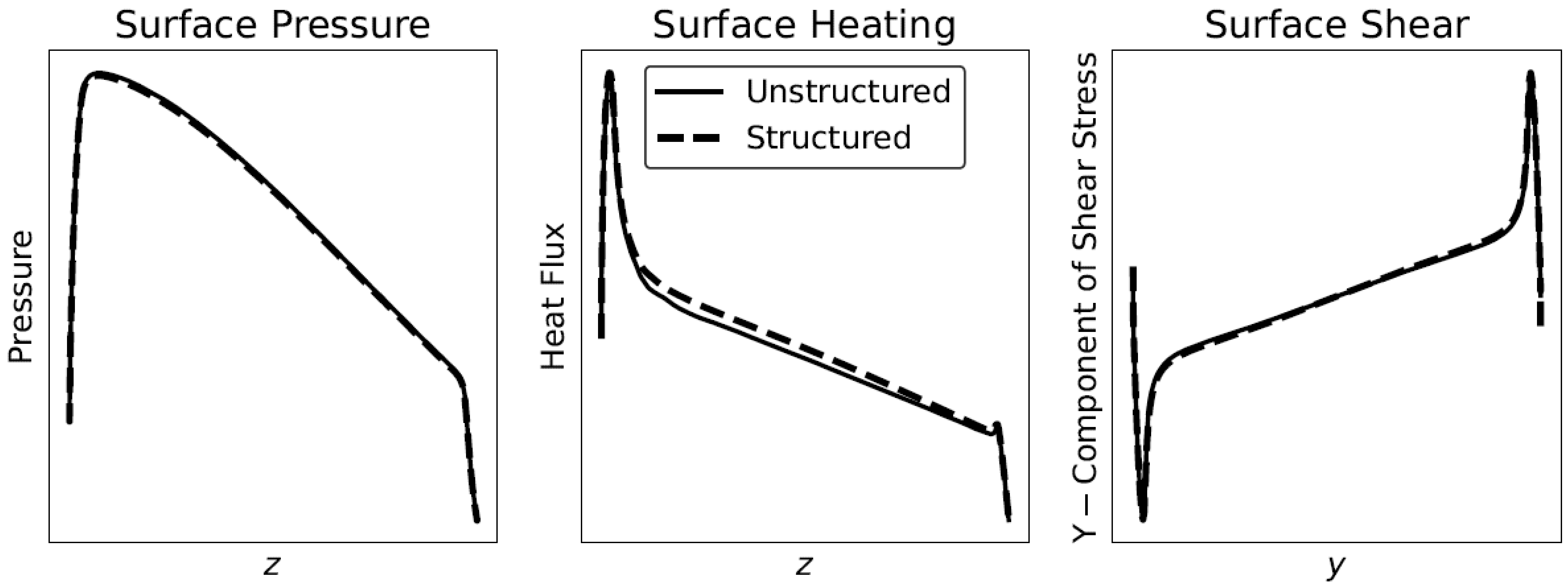
Hypersonic Flow over the Crew Exploration Vehicle (cont.)

Structured Grid | Unstructured Grid



Hypersonic Flow over the Crew Exploration Vehicle (cont.)

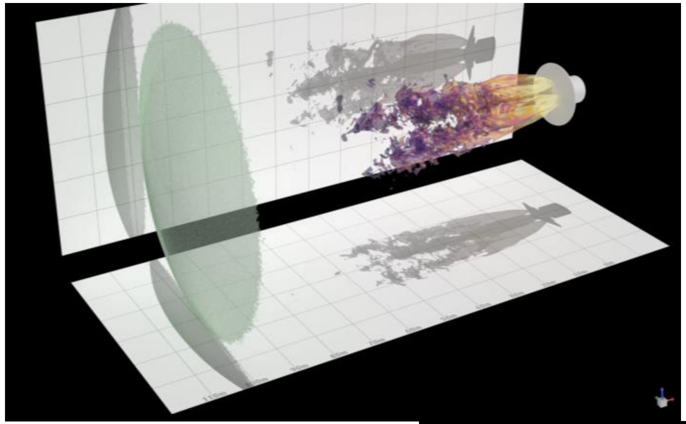
Centerline Surface Quantities



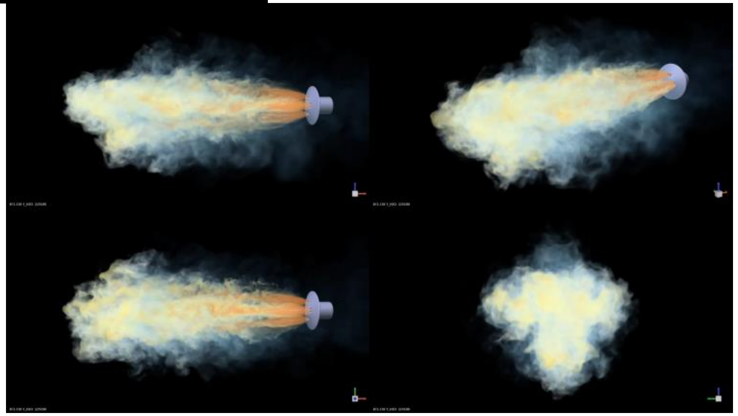
Peak stagnation heat transfer within 0.3%, Drag within 0.7%

Computational Performance
The Return of Desktop Computing?

- On the high end, FUN3D has demonstrated the ability to run at scale[1,2]
- Initial grids for all the simulations in this work took a few minutes to generate using DOD Capstone on a laptop
- **These adapted cases presented thus far were run on a workstation consisting of a single NVIDIA A100 80GB GPU and dual-socket AMD EPYC 7662 64-core CPUs**
  - High enthalpy hypersonic hemisphere cylinder: 5.5 hours
  - Hypersonic CEV: 10 hours
- In terms of performance, for generic gas path, the A100 80GB GPU is roughly equivalent to 7 AMD EPYC dual-socket nodes (896 cores)
- refine and I/O account for a third of this total runtime:
  - refine currently runs on the CPU only
  - If refine is ported to GPUs and refinement occurs internal to FUN3D, this percentage could be reduced further
- Perfect gas simulations are considerably cheaper
- **In this work, iteration and grid point strategies have not been optimized**



Isosurfaces of shock switch and H_2O mass fraction



Volume rendering of H_2O mass fraction

Chemically Reacting Supersonic Retropropulsion Mars Concept simulation on 16k~ V100s on ORNL Summit

[1] Korzun, A., Nastac, G., Walden, A., Nielsen, E. J., Jones, W., and Moran, P., “Application of a Detached Eddy Simulation Approach with Finite-Rate Chemistry to Mars-Relevant Retropropulsion Operating Environments,” AIAA SciTech 2022 Forum, 2022.

[2] Nastac, G., Korzun, A., Walden, A., Nielsen, E. J., Jones, W., and Moran, P., “Computational Investigation of the Effect of Chemistry on Mars Supersonic Retropropulsion Environments,” AIAA SciTech 2022 Forum, 2022.

Summary and Future Work

- Algorithmic flux improvements to FUN3D have been performed
- An adaptive mixed-element unstructured grid approach has been demonstrated
- Results have been demonstrated for realistic blunt bodies of interests with favorable comparisons to theory, experimental data, and structured grid results
- **The unstructured adapted grids produce comparable results to hand-crafted structured grids**
- **Combined with the GPU version of FUN3D, design cycles and database generation can occur more quickly for less cost**
- Extension of refine and Sketch-to-Solution to support mixed-element grids will further automate the gridding process